

3-BROMOPROPIONALDEHYDE DIMETHYL ACETAL

Other names:	Propane, 3-bromo-1,1-dimethoxy- 3-bromo-1,1-dimethoxypropane
Inchi:	InChI=1S/C5H11BrO2/c1-7-5(8-2)3-4-6/h5H,3-4H2,1-2H3
InchiKey:	ODZZAIFAQLODKN-UHFFFAOYSA-N
Formula:	C5H11BrO2
SMILES:	COC(CCB _r)OC
Mol. weight [g/mol]:	183.05

Physical Properties

Property code	Value	Unit	Source
hf	-397.77	kJ/mol	Cheméo Relay (1.0)
hfus	12.84	kJ/mol	Joback Method
hvap	49.26	kJ/mol	Cheméo Relay (1.0)
log10ws	-0.50		Cheméo Relay (1.0)
logp	1.390		Crippen Method
mcvol	110.550	ml/mol	McGowan Method
tb	449.06	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.86	J/mol×K	424.36	Joback Method
cpg	213.04	J/mol×K	455.83	Joback Method
cpg	221.95	J/mol×K	487.30	Joback Method
cpg	230.57	J/mol×K	518.77	Joback Method
cpg	238.91	J/mol×K	550.24	Joback Method
cpg	246.96	J/mol×K	581.72	Joback Method
cpg	254.72	J/mol×K	613.19	Joback Method
dvisc	0.0032665	Pa×s	235.37	Joback Method
dvisc	0.0016615	Pa×s	266.87	Joback Method
dvisc	0.0009748	Pa×s	298.37	Joback Method
dvisc	0.0006332	Pa×s	329.87	Joback Method
dvisc	0.0004435	Pa×s	361.36	Joback Method
dvisc	0.0003288	Pa×s	392.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.20	K	2.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36255444&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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